Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.80e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.92e-01

Confidence level: 6.08e-01

Nearest Neighbors from the Training Set

Image not found
Linoleic acid
Measured: 4.00e-02
Predicted: 6.98e-07

Image not found
Chloroacetyl chloride
Measured: 3.78e-02
Predicted: 33.9

Image not found
1,2-Diaminopropane
Measured: 7.00e-03
Predicted: 5.83

Image not found
Methylene iodide
Measured: 6.10e-02
Predicted: 2.52

Image not found
Ethane-1,2-dithiol
Measured: 3.91e-03
Predicted: 3.98